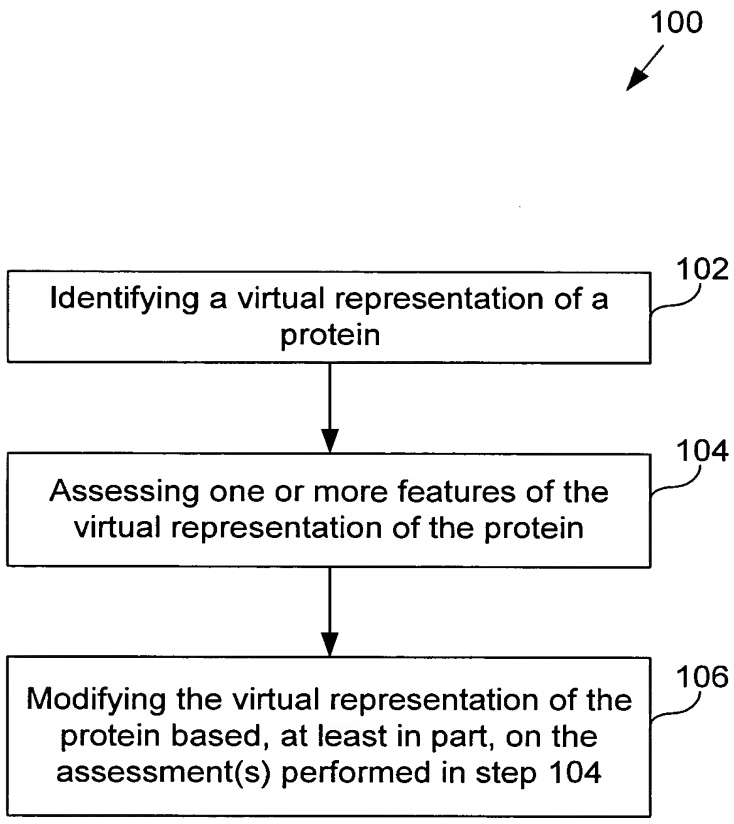


FIG. 1

0203-73.vsd/1

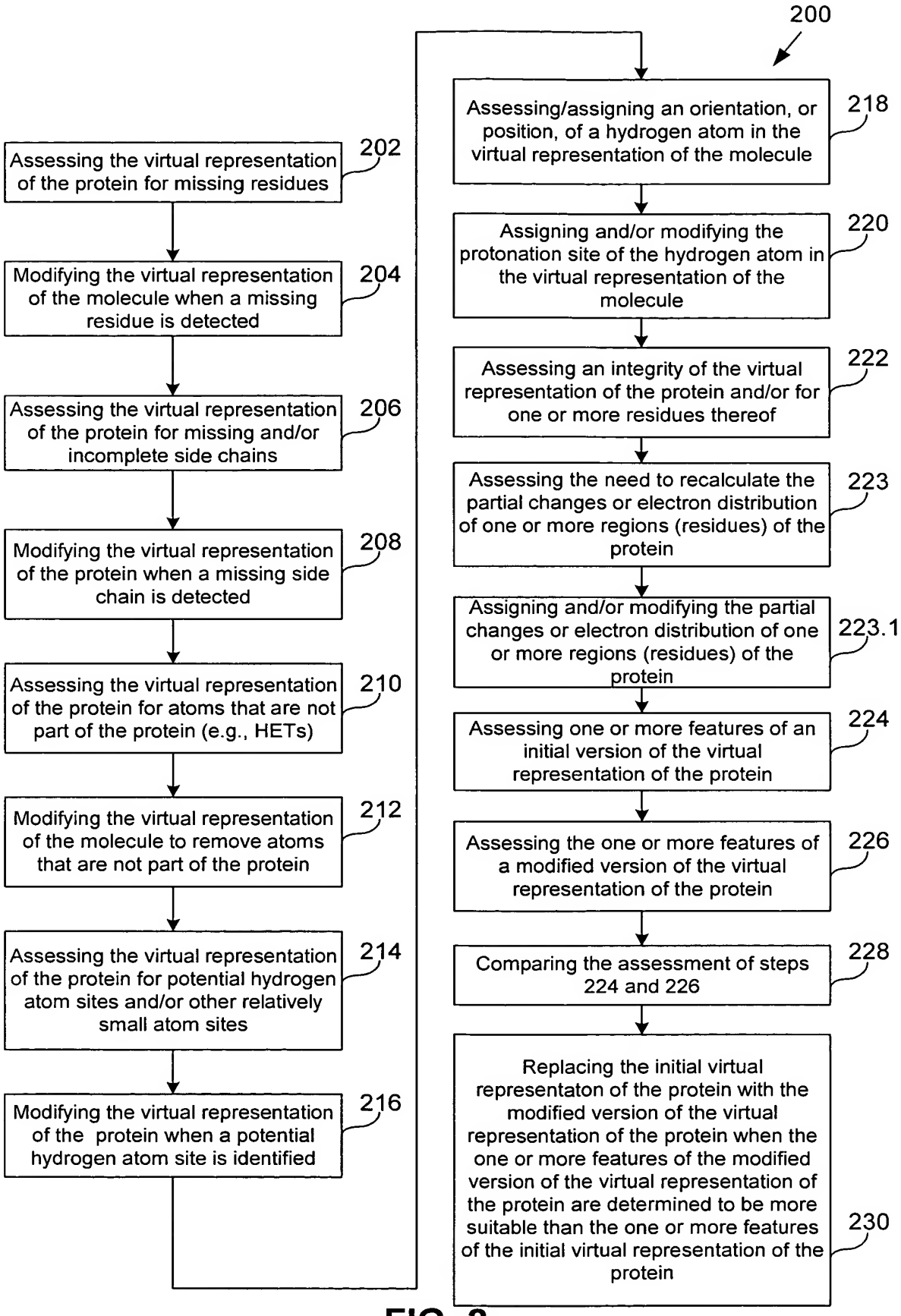


FIG. 2

0203-73.vsd/2

FIG. 3A

PDB
PROTEIN DATA BANK

Structure Explorer - 1AIK

[redacted]

Title **Hiv Gp41 Core Structure**
Classification **Glycoprotein**
Compound **Mol_Id: 1; Molecule: Hiv-1 Gp41 Glycoprotein; Chain: N, C; Fragment: Protease-Resistant Core; Biological_Unit: Trimer; Other_Details: N36 and C34 Are Synthetic Peptides**
Exp. Method **X-ray Diffraction**

Download/Display File

Summary Information
View Structure
Download/Display File
Structural Neighbors
Geometry
Other Sources
Sequence Details

[redacted]
SearchLite SearchFields

Save full entry to disk

```
HEADER    GLYCOPROTEIN                                20-APR-97   1AIK
TITLE     HIV GP41 CORE STRUCTURE
COMPND    MOL_ID: 1;
COMPND   2 MOLECULE: HIV-1 GP41 GLYCOPROTEIN;
COMPND   3 CHAIN: N, C;
COMPND   4 FRAGMENT: PROTEASE-RESISTANT CORE;
COMPND   5 BIOLOGICAL_UNIT: TRIMER;
COMPND   6 OTHER_DETAILS: N36 AND C34 ARE SYNTHETIC PEPTIDES
SOURCE    MOL_ID: 1;
SOURCE   2 ORGANISM_SCIENTIFIC: HUMAN IMMUNODEFICIENCY VIRUS TYPE 1;
SOURCE   3 STRAIN: HXB2;
SOURCE   4 CELLULAR_LOCATION: VIRAL MEMBRANE
KEYWDS    HIV, GP41, ENVELOPE GLYCOPROTEIN, RETROVIRUS
EXPDTA    X-RAY DIFFRACTION
AUTHOR    D.C.CHAN,D.FASS,J.M.BERGER,P.S.KIM
REVDAT   1   16-JUN-97 1AIK    0
REMARK    1
REMARK   1 REFERENCE 1
REMARK   1  AUTH    D.C.CHAN,D.FASS,J.M.BERGER,P.S.KIM
REMARK   1  TITL    CORE STRUCTURE OF GP41 FROM THE HIV ENVELOPE
REMARK   1  TITL 2 GLYCOPROTEIN
REMARK   1  REF     CELL(CAMBRIDGE,MASS.)          V.  89    263 1997
REMARK   1  REFN    ASTM CELLB5  US ISSN 0092-8674                  0998
REMARK    2
REMARK   2 RESOLUTION. 2.0  ANGSTROMS.
REMARK    3
REMARK   3 REFINEMENT.
REMARK   3   PROGRAM     : X-PLOR 3.851
```

```
REMARK   3   AUTHORS     : BRUNGER
REMARK   3
REMARK   3  DATA USED IN REFINEMENT.
REMARK   3   RESOLUTION RANGE HIGH (ANGSTROMS) : 2.0
REMARK   3   RESOLUTION RANGE LOW  (ANGSTROMS) : 12.0
REMARK   3   DATA CUTOFF            (SIGMA(F)) : 2.0
REMARK   3   DATA CUTOFF HIGH         (ABS(F)) : 100000000.
REMARK   3   DATA CUTOFF LOW          (ABS(F)) : NULL
REMARK   3   COMPLETENESS (WORKING+TEST)   (%) : 96.5
REMARK   3   NUMBER OF REFLECTIONS             : 5683
REMARK   3
REMARK   3  FIT TO DATA USED IN REFINEMENT.
REMARK   3   CROSS-VALIDATION METHOD           : THROUGHOUT
REMARK   3   FREE R VALUE TEST SET SELECTION   : RANDOM
REMARK   3   R VALUE            (WORKING SET) : 0.238
REMARK   3   FREE R VALUE                      : 0.266
REMARK   3   FREE R VALUE TEST SET SIZE   (%) : 7.12
REMARK   3   FREE R VALUE TEST SET COUNT       : 371
REMARK   3   ESTIMATED ERROR OF FREE R VALUE   : NULL
REMARK   3
REMARK   3  FIT IN THE HIGHEST RESOLUTION BIN.
REMARK   3   TOTAL NUMBER OF BINS USED           : NULL
REMARK   3   BIN RESOLUTION RANGE HIGH       (A) : NULL
REMARK   3   BIN RESOLUTION RANGE LOW        (A) : NULL
REMARK   3   BIN COMPLETENESS (WORKING+TEST) (%) : NULL
REMARK   3   REFLECTIONS IN BIN    (WORKING SET) : NULL
REMARK   3   BIN R VALUE           (WORKING SET) : NULL
REMARK   3   BIN FREE R VALUE                    : NULL
REMARK   3   BIN FREE R VALUE TEST SET SIZE  (%) : NULL
REMARK   3   BIN FREE R VALUE TEST SET COUNT     : NULL
REMARK   3   ESTIMATED ERROR OF BIN FREE R VALUE : NULL
REMARK   3
REMARK   3  NUMBER OF NON-HYDROGEN ATOMS USED IN REFINEMENT.
REMARK   3   PROTEIN ATOMS            : 596
REMARK   3   NUCLEIC ACID ATOMS       : 0
REMARK   3   HETEROGEN ATOMS          : 0
REMARK   3   SOLVENT ATOMS            : 43
REMARK   3
REMARK   3  B VALUES.
REMARK   3   FROM WILSON PLOT           (A**2) : NULL
REMARK   3   MEAN B VALUE      (OVERALL, A**2) : NULL
REMARK   3   OVERALL ANISOTROPIC B VALUE.
REMARK   3    B11 (A**2) : NULL
```

FIG. 3C


```
REMARK   3    B22 (A**2) : NULL
REMARK   3    B33 (A**2) : NULL
REMARK   3    B12 (A**2) : NULL
REMARK   3    B13 (A**2) : NULL
REMARK   3    B23 (A**2) : NULL
REMARK   3
REMARK   3  ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM LUZZATI PLOT          (A) : NULL
REMARK   3   ESD FROM SIGMAA                (A) : NULL
REMARK   3   LOW RESOLUTION CUTOFF          (A) : NULL
REMARK   3
REMARK   3  CROSS-VALIDATED ESTIMATED COORDINATE ERROR.
REMARK   3   ESD FROM C-V LUZZATI PLOT      (A) : NULL
REMARK   3   ESD FROM C-V SIGMAA            (A) : NULL
REMARK   3
REMARK   3  RMS DEVIATIONS FROM IDEAL VALUES.
REMARK   3   BOND LENGTHS                   (A) : 0.014
REMARK   3   BOND ANGLES             (DEGREES) : 2.742
REMARK   3   DIHEDRAL ANGLES         (DEGREES) : NULL
REMARK   3   IMPROPER ANGLES         (DEGREES) : NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL MODEL : NULL
REMARK   3
REMARK   3  ISOTROPIC THERMAL FACTOR RESTRAINTS.     RMS     SIGMA
REMARK   3   MAIN-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   MAIN-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN BOND              (A**2) : NULL  ; NULL
REMARK   3   SIDE-CHAIN ANGLE             (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  NCS MODEL : NULL
REMARK   3
REMARK   3  NCS RESTRAINTS.                          RMS   SIGMA/WEIGHT
REMARK   3   GROUP  1  POSITIONAL              (A) : NULL  ; NULL
REMARK   3   GROUP  1  B-FACTOR            (A**2) : NULL  ; NULL
REMARK   3
REMARK   3  PARAMETER FILE  1  : NULL
REMARK   3  PARAMETER FILE  2  : NULL
REMARK   3  TOPOLOGY FILE  1   : NULL
REMARK   3  TOPOLOGY FILE  2   : NULL
REMARK   3
REMARK   3  OTHER REFINEMENT REMARKS: NULL
REMARK   4
REMARK   4 1AIK COMPLIES WITH FORMAT V. 2.2, 16-DEC-1996
```

FIG. 3D


```
REMARK   6
REMARK   6 C-TERMINAL NH2 NOT IN ATOM LIST FOR BOTH CHAINS.
REMARK 200
REMARK 200 EXPERIMENTAL DETAILS
REMARK 200  EXPERIMENT TYPE                : X-RAY DIFFRACTION
REMARK 200  DATE OF DATA COLLECTION        : MAR-1997
REMARK 200  TEMPERATURE           (KELVIN) : 100
REMARK 200  PH                             : 6.0
REMARK 200  NUMBER OF CRYSTALS USED        : 1
REMARK 200
REMARK 200  SYNCHROTRON              (Y/N) : N
REMARK 200  RADIATION SOURCE               : NULL
REMARK 200  BEAMLINE                       : NULL
REMARK 200  X-RAY GENERATOR MODEL          : RIGAKU RU200
REMARK 200  MONOCHROMATIC OR LAUE    (M/L) : M
REMARK 200  WAVELENGTH OR RANGE        (A) : 1.5418
REMARK 200  MONOCHROMATOR                  : NULL
REMARK 200  OPTICS                         : MIRRORS
REMARK 200
REMARK 200  DETECTOR TYPE                  : R-AXIS IIC
REMARK 200  DETECTOR MANUFACTURER          : RIGAKU
REMARK 200  INTENSITY-INTEGRATION SOFTWARE : DENZO
REMARK 200  DATA SCALING SOFTWARE          : SCALEPACK
REMARK 200
REMARK 200  NUMBER OF UNIQUE REFLECTIONS   : 5287
REMARK 200  RESOLUTION RANGE HIGH      (A) : 2.0
REMARK 200  RESOLUTION RANGE LOW       (A) : 20.0
REMARK 200  REJECTION CRITERIA  (SIGMA(I)) : 1.5
REMARK 200
REMARK 200 OVERALL.
REMARK 200  COMPLETENESS FOR RANGE     (%) : 96.5
REMARK 200  DATA REDUNDANCY                : NULL
REMARK 200  R MERGE                    (I) : NULL
REMARK 200  R SYM                      (I) : 0.054
REMARK 200  <I/SIGMA(I)> FOR THE DATA SET  : 18.4
REMARK 200
REMARK 200 IN THE HIGHEST RESOLUTION SHELL.
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE HIGH (A) : 2.00
REMARK 200  HIGHEST RESOLUTION SHELL, RANGE LOW  (A) : 2.07
REMARK 200  COMPLETENESS FOR SHELL     (%) : 98.9
REMARK 200  DATA REDUNDANCY IN SHELL       : NULL
REMARK 200  R MERGE FOR SHELL          (I) : NULL
REMARK 200  R SYM FOR SHELL            (I) : 0.263
```

FIG. 3E


```
REMARK 200  <I/SIGMA(I)> FOR SHELL         : 5.4
REMARK 200
REMARK 200 METHOD USED TO DETERMINE THE STRUCTURE: MAD
REMARK 200 SOFTWARE USED: CCP4 SUITE
REMARK 200 STARTING MODEL: NULL
REMARK 200
REMARK 200 REMARK: DATA AT NSLS USED MAD METHODS.  DATA COLLECTED ON
REMARK 200 AN OSMIUM-SOAK CRYSTAL AT WAVELENGTHS 1.1398, 1.1396,
REMARK 200 1.1344, AND 1.1406 ANGSTROMS.
REMARK 280
REMARK 280 CRYSTAL
REMARK 280 SOLVENT CONTENT, VS   (%): 46.
REMARK 280 MATTHEWS COEFFICIENT, VM (ANGSTROMS**3/DA): NULL
REMARK 280
REMARK 280 CRYSTALLIZATION CONDITIONS: A 10 MG/ML STOCK WAS DILUTED
REMARK 280 1:1 IN A SITTING DROP WITH 80 MM NH4CL, 20% PEG200, AND
REMARK 280 50% ISOPROPANOL, AND THEN ALLOWED TO EQUILIBRATE AGAINST
REMARK 280 80 MM NH4CL, 20% PEG200, AND 30% ISOPROPANOL.
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY
REMARK 290 SYMMETRY OPERATORS FOR SPACE GROUP: P 3 2 1
REMARK 290
REMARK 290      SYMOP   SYMMETRY
REMARK 290     NNNMMM   OPERATOR
REMARK 290       1555   X,Y,Z
REMARK 290       2555   -Y,X-Y,Z
REMARK 290       3555   Y-X,-X,Z
REMARK 290       4555   Y,X,-Z
REMARK 290       5555   X-Y,-Y,-Z
REMARK 290       6555   -X,Y-X,-Z
REMARK 290
REMARK 290     WHERE NNN -> OPERATOR NUMBER
REMARK 290           MMM -> TRANSLATION VECTOR
REMARK 290
REMARK 290 CRYSTALLOGRAPHIC SYMMETRY TRANSFORMATIONS
REMARK 290 THE FOLLOWING TRANSFORMATIONS OPERATE ON THE ATOM/HETATM
REMARK 290 RECORDS IN THIS ENTRY TO PRODUCE CRYSTALLOGRAPHICALLY
REMARK 290 RELATED MOLECULES.
REMARK 290   SMTRY1   1  1.000000  0.000000  0.000000        0.00000
REMARK 290   SMTRY2   1  0.000000  1.000000  0.000000        0.00000
REMARK 290   SMTRY3   1  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   2 -0.500021 -0.866016  0.000000        0.00000
REMARK 290   SMTRY2   2  0.866035 -0.499979  0.000000        0.00000
```

FIG. 3F

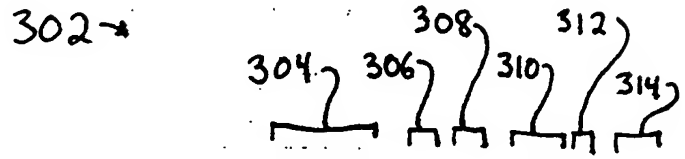

```
REMARK 290   SMTRY3   2  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   3 -0.499979  0.866016  0.000000        0.00000
REMARK 290   SMTRY2   3 -0.866035 -0.500021  0.000000        0.00000
REMARK 290   SMTRY3   3  0.000000  0.000000  1.000000        0.00000
REMARK 290   SMTRY1   4 -0.500021  0.865991  0.000000        0.00000
REMARK 290   SMTRY2   4  0.866035  0.500021  0.000000        0.00000
REMARK 290   SMTRY3   4  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   5  1.000000  0.000050  0.000000        0.00000
REMARK 290   SMTRY2   5  0.000000 -1.000000  0.000000        0.00000
REMARK 290   SMTRY3   5  0.000000  0.000000 -1.000000        0.00000
REMARK 290   SMTRY1   6 -0.499979 -0.866041  0.000000        0.00000
REMARK 290   SMTRY2   6 -0.866035  0.499979  0.000000        0.00000
REMARK 290   SMTRY3   6  0.000000  0.000000 -1.000000        0.00000
REMARK 290
REMARK 290 REMARK: NULL
REMARK 999
REMARK 999 SEQUENCE
REMARK 999 1AIK  C    SWS     P04582       1 -   621 NOT IN ATOMS LIST
REMARK 999 1AIK  C    SWS     P04582     657 -   851 NOT IN ATOMS LIST
REMARK 999 1AIK  N    SWS     P19551       1 -   542 NOT IN ATOMS LIST
REMARK 999 1AIK  N    SWS     P19551     580 -   853 NOT IN ATOMS LIST
DBREF  1AIK C    0   661  SWS    P04582   ENV_HV1B8      622    656
DBREF  1AIK N    0   581  SWS    P19551   ENV_HV1MF      543    579
SEQADV 1AIK ACE C    0  SWS  P04582    THR   622 CONFLICT
SEQADV 1AIK ACE N    0  SWS  P19551    LEU   543 CONFLICT
SEQRES   1 N   38  ACE SER GLY ILE VAL GLN GLN GLN ASN ASN LEU LEU ARG
SEQRES   2 N   38  ALA ILE GLU ALA GLN GLN HIS LEU LEU GLN LEU THR VAL
SEQRES   3 N   38  TRP GLY ILE LYS GLN LEU GLN ALA ARG ILE LEU NH2
SEQRES   1 C   36  ACE TRP MET GLU TRP ASP ARG GLU ILE ASN ASN TYR THR
SEQRES   2 C   36  SER LEU ILE HIS SER LEU ILE GLU GLU SER GLN ASN GLN
SEQRES   3 C   36  GLN GLU LYS ASN GLU GLN GLU LEU LEU NH2
HET    ACE  N   0       3
HET    ACE  C   0       3
HETNAM     ACE ACETYL GROUP
FORMUL   1  ACE    C2 H3 O1
FORMUL   2  ACE    C2 H3 O1
FORMUL   3  HOH   *43(H2 O1)
HELIX    1   1 GLY N  547  ALA N  578  1                                  32
HELIX    2   2 MET C  629  GLU C  659  1                                  31
LINK         C   ACE N   0                 N   SER N 546
LINK         C   ACE C   0                 N   TRP C 628
CRYST1   49.500   49.500   55.300  90.00  90.00 120.00 P 3 2 1       6
ORIGX1      1.000000  0.000000  0.000000        0.00000
```

FIG. 3G

302

```
ORIGX2      0.000000  1.000000  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000        0.00000
SCALE1      0.020202  0.011664  0.000000        0.00000
SCALE2      0.000000  0.023327  0.000000        0.00000
SCALE3      0.000000  0.000000  0.018083        0.00000
HETATM    1  C   ACE N   0      19.211  14.270 -17.472  1.00 56.26           C
HETATM    2  O   ACE N   0      19.488  14.580 -16.305  1.00 56.37           O
HETATM    3  CH3 ACE N   0      20.273  14.045 -18.531  1.00 56.01           C
ATOM      4  N   SER N 546      17.955  14.014 -17.827  1.00 56.49           N
ATOM      5  CA  SER N 546      16.876  14.392 -16.942  1.00 56.15           C
ATOM      6  C   SER N 546      16.909  13.631 -15.655  1.00 56.24           C
ATOM      7  O   SER N 546      16.736  14.255 -14.615  1.00 57.67           O
ATOM      8  CB  SER N 546      15.525  14.172 -17.546  1.00 56.05           C
ATOM      9  OG  SER N 546      15.498  12.815 -17.842  1.00 57.84           O
ATOM     10  H   SER N 546      17.816  13.501 -18.652  1.00  0.00           H
ATOM     11  HG  SER N 546      15.988  12.455 -18.582  1.00  0.00           H
ATOM     12  N   GLY N 547      17.181  12.316 -15.724  1.00 55.59           N
ATOM     13  CA  GLY N 547      17.202  11.414 -14.570  1.00 53.04           C
ATOM     14  C   GLY N 547      18.299  11.783 -13.596  1.00 51.70           C
ATOM     15  O   GLY N 547      18.147  11.667 -12.391  1.00 50.76           O
ATOM     16  H   GLY N 547      17.409  11.945 -16.618  1.00  0.00           H
ATOM     17  N   ILE N 548      19.399  12.280 -14.145  1.00 51.57           N
ATOM     18  CA  ILE N 548      20.551  12.815 -13.425  1.00 52.14           C
ATOM     19  C   ILE N 548      20.218  14.116 -12.696  1.00 51.31           C
ATOM     20  O   ILE N 548      20.543  14.273 -11.519  1.00 50.83           O
ATOM     21  CB  ILE N 548      21.693  13.043 -14.436  1.00 54.22           C
ATOM     22  CG1 ILE N 548      22.120  11.712 -15.087  1.00 54.58           C
ATOM     23  CG2 ILE N 548      22.861  13.705 -13.721  1.00 55.25           C
ATOM     24  CD1 ILE N 548      23.126  11.909 -16.234  1.00 56.29           C
ATOM     25  H   ILE N 548      19.445  12.272 -15.118  1.00  0.00           H
ATOM     26  N   VAL N 549      19.590  15.054 -13.393  1.00 50.93           N
ATOM     27  CA  VAL N 549      19.093  16.291 -12.786  1.00 50.79           C
ATOM     28  C   VAL N 549      18.036  15.977 -11.726  1.00 50.36           C
ATOM     29  O   VAL N 549      17.992  16.598 -10.674  1.00 51.60           O
ATOM     30  CB  VAL N 549      18.451  17.196 -13.841  1.00 52.28           C
ATOM     31  CG1 VAL N 549      17.814  18.437 -13.226  1.00 54.97           C
ATOM     32  CG2 VAL N 549      19.539  17.650 -14.780  1.00 51.05           C
ATOM     33  H   VAL N 549      19.486  14.911 -14.360  1.00  0.00           H
ATOM     34  N   GLN N 550      17.187  15.030 -12.001  1.00 49.13           N
ATOM     35  CA  GLN N 550      16.176  14.508 -11.109  1.00 49.23           C
ATOM     36  C   GLN N 550      16.843  13.895  -9.861  1.00 48.50           C
ATOM     37  O   GLN N 550      16.520  14.236  -8.736  1.00 47.94           O
ATOM     38  CB  GLN N 550      15.452  13.398 -11.814  1.00 52.96           C
```

FIG. 3H



HETATM	1	C	ACE	N	0	19.211	14.270	-17.472	1.00	56.26
HETATM	2	O	ACE	N	0	19.488	14.580	-16.305	1.00	56.37
HETATM	3	CH3	ACE	N	0	20.273	14.045	-18.531	1.00	56.01
ATOM	4	N	SER	N	546	17.955	14.014	-17.827	1.00	56.49
ATOM	5	CA	SER	N	546	16.876	14.392	-16.942	1.00	56.15
ATOM	6	C	SER	N	546	16.909	13.631	-15.655	1.00	56.24
ATOM	7	O	SER	N	546	16.736	14.255	-14.615	1.00	57.67
ATOM	8	CB	SER	N	546	15.525	14.172	-17.546	1.00	56.05
ATOM	9	OG	SER	N	546	15.498	12.815	-17.842	1.00	57.84
ATOM	10	H	SER	N	546	17.816	13.501	-18.652	1.00	0.00
ATOM	11	HG	SER	N	546	15.988	12.455	-18.582	1.00	0.00
ATOM	12	N	GLY	N	547	17.181	12.316	-15.724	1.00	55.59
ATOM	13	CA	GLY	N	547	17.202	11.414	-14.570	1.00	53.04
ATOM	14	C	GLY	N	547	18.299	11.783	-13.596	1.00	51.70
ATOM	15	O	GLY	N	547	18.147	11.667	-12.391	1.00	50.76
ATOM	16	H	GLY	N	547	17.409	11.945	-16.618	1.00	0.00
ATOM	17	N	ILE	N	548	19.399	12.280	-14.145	1.00	51.57
ATOM	18	CA	ILE	N	548	20.551	12.815	-13.425	1.00	52.14
ATOM	19	C	ILE	N	548	20.218	14.116	-12.696	1.00	51.31
ATOM	20	O	ILE	N	548	20.543	14.273	-11.519	1.00	50.83
ATOM	21	CB	ILE	N	548	21.693	13.043	-14.436	1.00	54.22
ATOM	22	CG1	ILE	N	548	22.120	11.712	-15.087	1.00	54.58
ATOM	23	CG2	ILE	N	548	22.861	13.705	-13.721	1.00	55.25
ATOM	24	CD1	ILE	N	548	23.126	11.909	-16.234	1.00	56.29
ATOM	25	H	ILE	N	548	19.445	12.272	-15.118	1.00	0.00
ATOM	26	N	VAL	N	549	19.590	15.054	-13.393	1.00	50.93
ATOM	27	CA	VAL	N	549	19.093	16.291	-12.786	1.00	50.79
ATOM	28	C	VAL	N	549	18.036	15.977	-11.726	1.00	50.36
ATOM	29	O	VAL	N	549	17.992	16.598	-10.674	1.00	51.60
ATOM	30	CB	VAL	N	549	18.451	17.196	-13.841	1.00	52.28
ATOM	31	CG1	VAL	N	549	17.814	18.437	-13.226	1.00	54.97
ATOM	32	CG2	VAL	N	549	19.539	17.650	-14.780	1.00	51.05
ATOM	33	H	VAL	N	549	19.486	14.911	-14.360	1.00	0.00
ATOM	34	N	GLN	N	550	17.187	15.030	-12.001	1.00	49.13
ATOM	35	CA	GLN	N	550	16.176	14.508	-11.109	1.00	49.23
ATOM	36	C	GLN	N	550	16.843	13.895	-9.861	1.00	48.50
ATOM	37	O	GLN	N	550	16.520	14.236	-8.736	1.00	47.94
ATOM	38	CB	GLN	N	550	15.452	13.398	-11.814	1.00	52.96

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REMARK 987       26.67       25.42       53.56
ATOM      1   C   ACE A   0      -5.539   -0.020  -17.472
ATOM      2   O   ACE A   0      -5.262    0.290  -16.305
ATOM      3   CH3 ACE A   0      -4.477   -0.245  -18.531
ATOM      4 1HH3 ACE A   0      -3.490   -0.091  -18.094
ATOM      5 2HH3 ACE A   0      -4.626    0.459  -19.350
ATOM      6 3HH3 ACE A   0      -4.552   -1.264  -18.910
ATOM      7   N   SER A 546      -6.795   -0.276  -17.827
ATOM      8   CA  SER A 546      -7.874    0.102  -16.942
ATOM      9   C   SER A 546      -7.841   -0.659  -15.655
ATOM     10   O   SER A 546      -8.014   -0.035  -14.615
ATOM     11   CB  SER A 546      -9.225   -0.118  -17.546
ATOM     12   OG  SER A 546      -9.252   -1.475  -17.842
ATOM     13   H   SER A 546      -6.993   -0.730  -18.707
ATOM     14   HA  SER A 546      -7.718    1.166  -16.762
ATOM     15   HB2 SER A 546      -9.345    0.477  -18.451
ATOM     16   HB3 SER A 546     -10.012    0.138  -16.836
ATOM     17   HG  SER A 546     -10.097   -1.699  -18.238
ATOM     18   N   GLY A 547      -7.569   -1.974  -15.724
ATOM     19   CA  GLY A 547      -7.548   -2.876  -14.570
ATOM     20   C   GLY A 547      -6.451   -2.507  -13.596
ATOM     21   O   GLY A 547      -6.603   -2.623  -12.391
ATOM     22   H   GLY A 547      -7.365   -2.366  -16.632
ATOM     23   HA2 GLY A 547      -7.382   -3.895  -14.920
ATOM     24   HA3 GLY A 547      -8.509   -2.819  -14.059
ATOM     25   N   ILE A 548      -5.351   -2.010  -14.145
ATOM     26   CA  ILE A 548      -4.199   -1.475  -13.425
ATOM     27   C   ILE A 548      -4.532   -0.174  -12.696
ATOM     28   O   ILE A 548      -4.207   -0.017  -11.519
ATOM     29   CB  ILE A 548      -3.057   -1.247  -14.436
ATOM     30   CG1 ILE A 548      -2.630   -2.578  -15.087
ATOM     31   CG2 ILE A 548      -1.889   -0.585  -13.721
ATOM     32   CD1 ILE A 548      -1.624   -2.381  -16.234
ATOM     33   H   ILE A 548      -5.306   -2.001  -15.154
ATOM     34   HA  ILE A 548      -3.897   -2.193  -12.663
ATOM     35   HB  ILE A 548      -3.403   -0.592  -15.236
ATOM     36 2HG1 ILE A 548      -3.517   -3.073  -15.482
ATOM     37 3HG1 ILE A 548      -2.171   -3.208  -14.325
ATOM     38 1HG2 ILE A 548      -1.076   -0.420  -14.429
ATOM     39 2HG2 ILE A 548      -1.543   -1.232  -12.915
ATOM     40 3HG2 ILE A 548      -2.211    0.371  -13.307
ATOM     41 1HD1 ILE A 548      -1.359   -3.351  -16.655
ATOM     42 2HD1 ILE A 548      -0.727   -1.893  -15.851
ATOM     43 3HD1 ILE A 548      -2.073   -1.759  -17.008
ATOM     44   N   VAL A 549      -5.160    0.764  -13.393
ATOM     45   CA  VAL A 549      -5.657    2.001  -12.786
ATOM     46   C   VAL A 549      -6.714    1.687  -11.726
ATOM     47   O   VAL A 549      -6.758    2.308  -10.674
ATOM     48   CB  VAL A 549      -6.299    2.906  -13.841
ATOM     49   CG1 VAL A 549      -6.936    4.147  -13.226
ATOM     50   CG2 VAL A 549      -5.211    3.360  -14.780
ATOM     51   H   VAL A 549      -5.301    0.619  -14.382
ATOM     52   HA  VAL A 549      -4.805    2.508  -12.333
ATOM     53   HB  VAL A 549      -7.080    2.340  -14.348
ATOM     54 1HG1 VAL A 549      -7.378    4.757  -14.014
ATOM     55 2HG1 VAL A 549      -6.174    4.725  -12.703
```

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FIG. 4

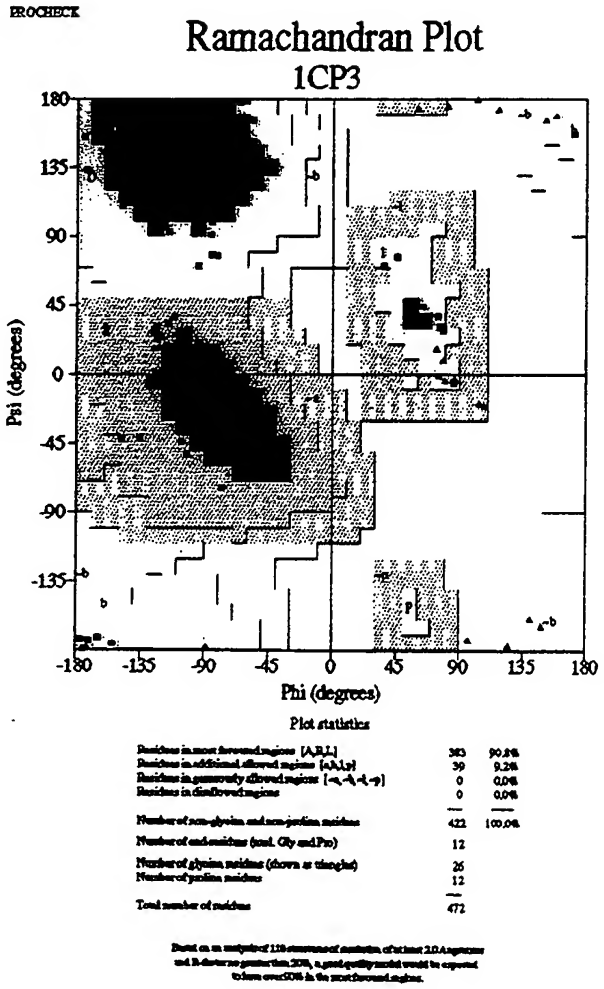

PROCHECK
Ramachandran Plot
1CP3
Psi (degrees)
Phi (degrees)
180
135
90
45
0
-45
-90
-135
-180
Plot statistics

FIG. 5A

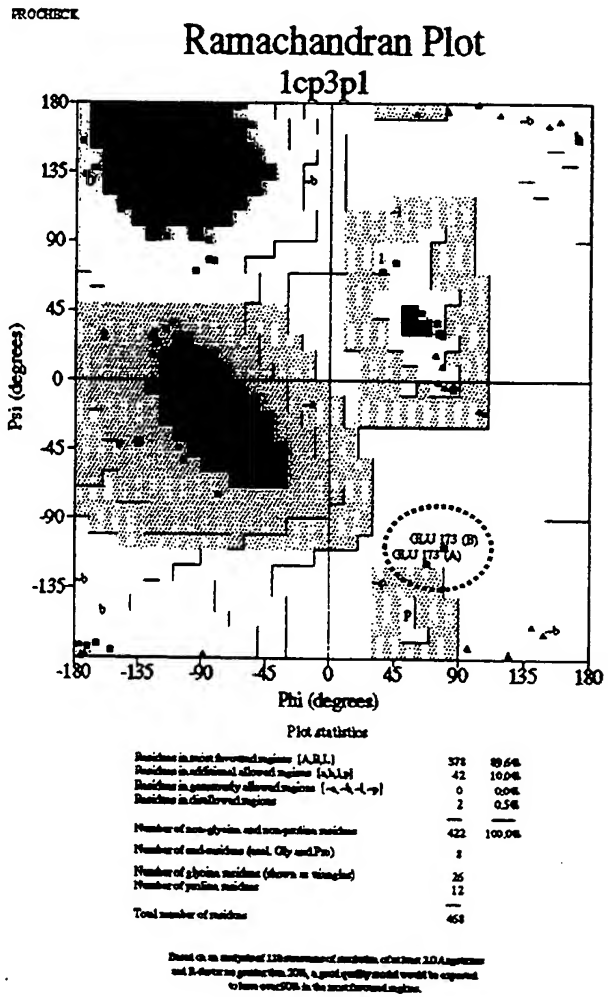

PROCHECK
Ramachandran Plot
1cp3p1
Psi (degrees)
Phi (degrees)
180
135
90
45
0
-45
-90
-135
-180
Plot statistics

FIG. 5B

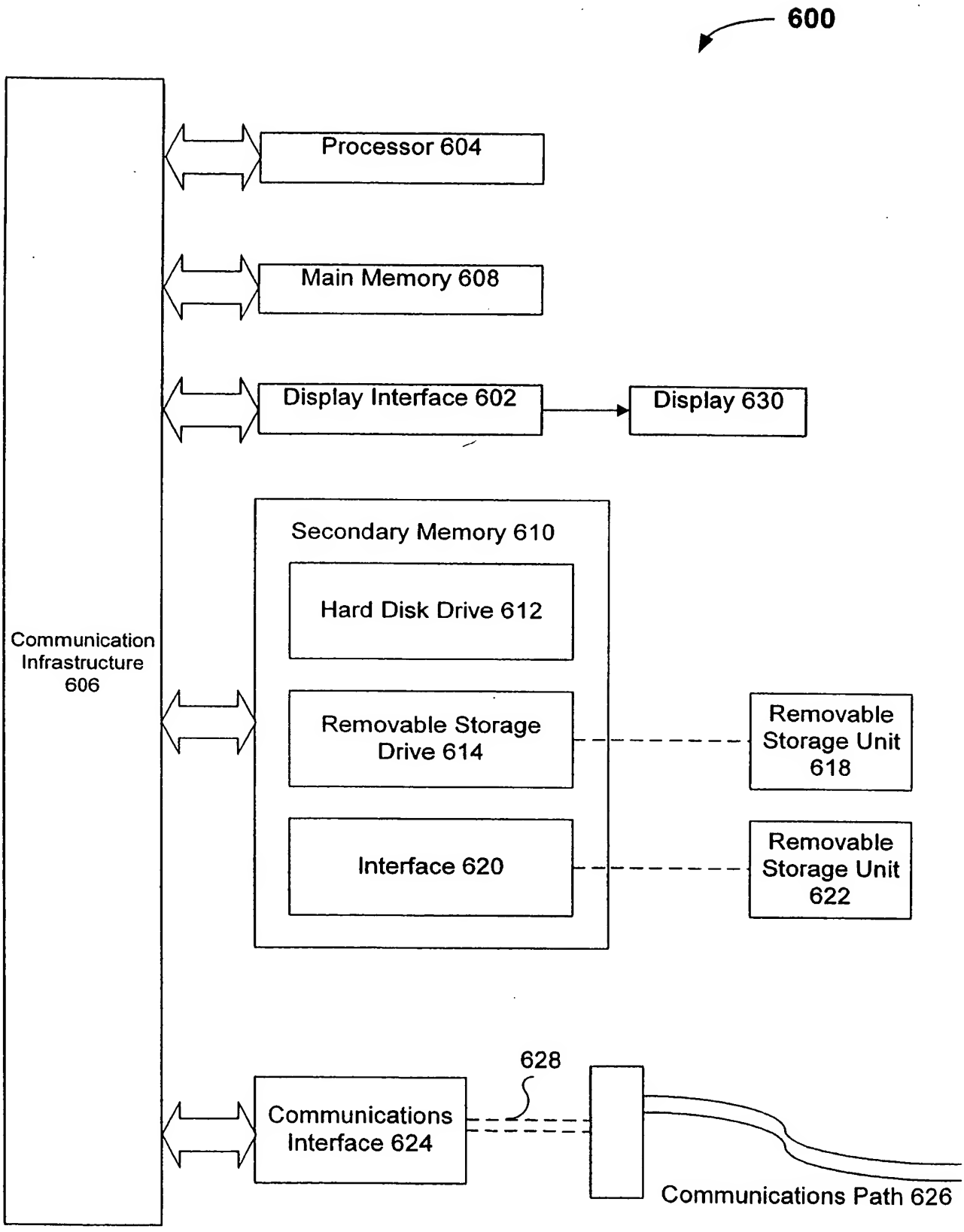


FIG. 6

computer.vsd/1

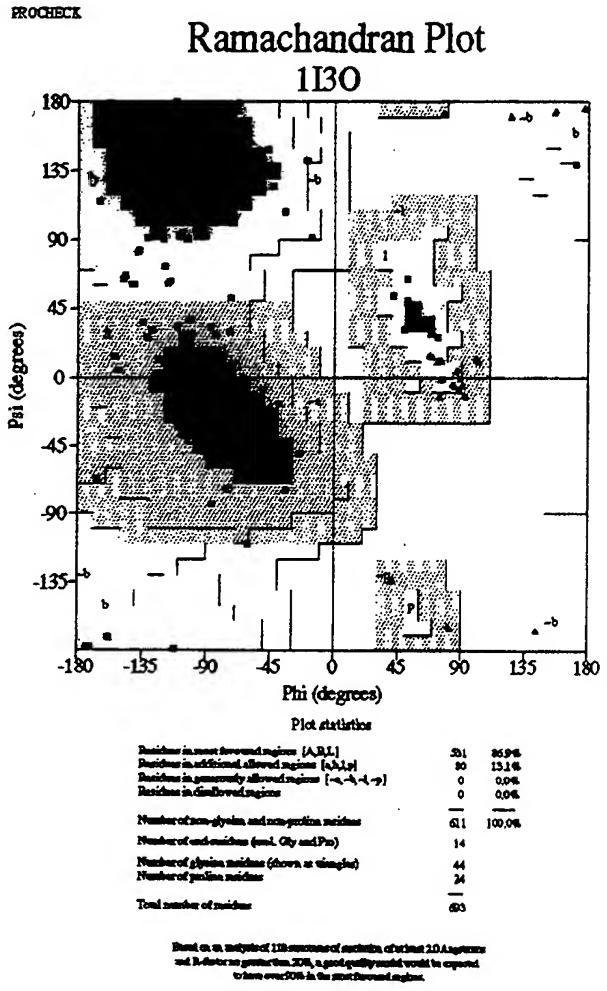

PROCHECK
Ramachandran Plot
1I3O
Psi (degrees)
Phi (degrees)
180
135
90
45
0
-45
-90
-135
-180
Plot statistics

FIG. 7A

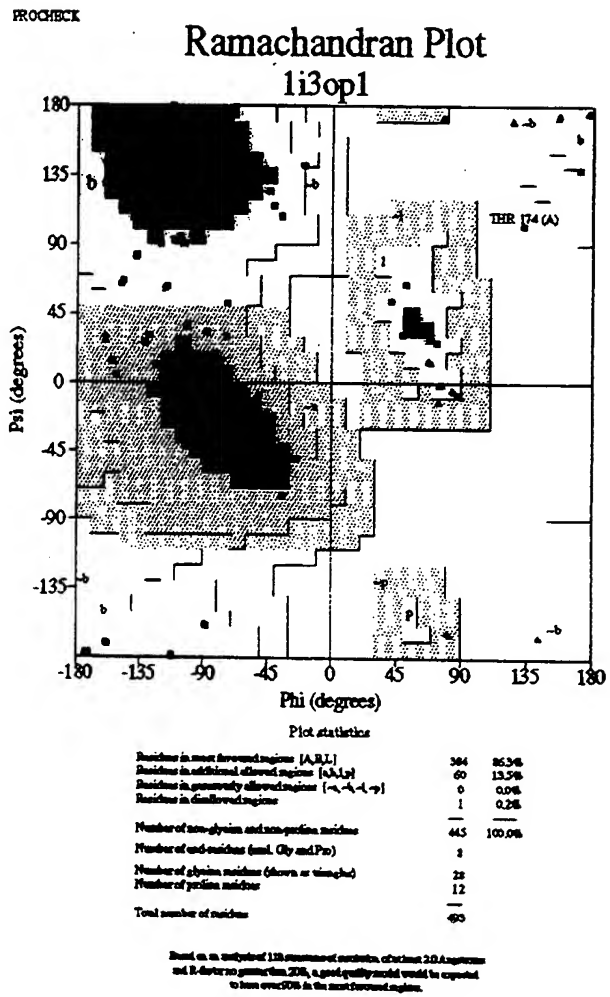

PROCHECK
Ramachandran Plot
1i3op1
THR 74 (A)
Psi (degrees)
Phi (degrees)
180
135
90
45
0
-45
-90
-135
-180
Plot statistics

FIG. 7B

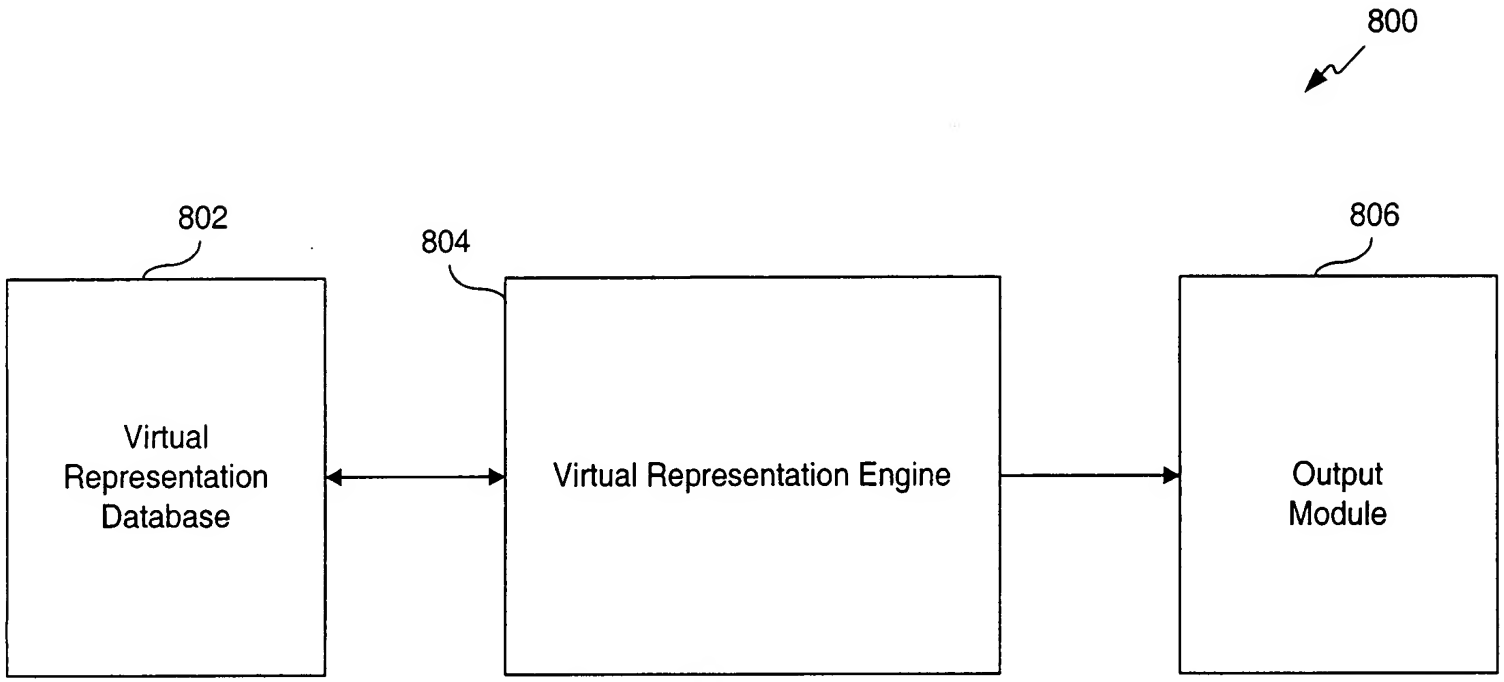
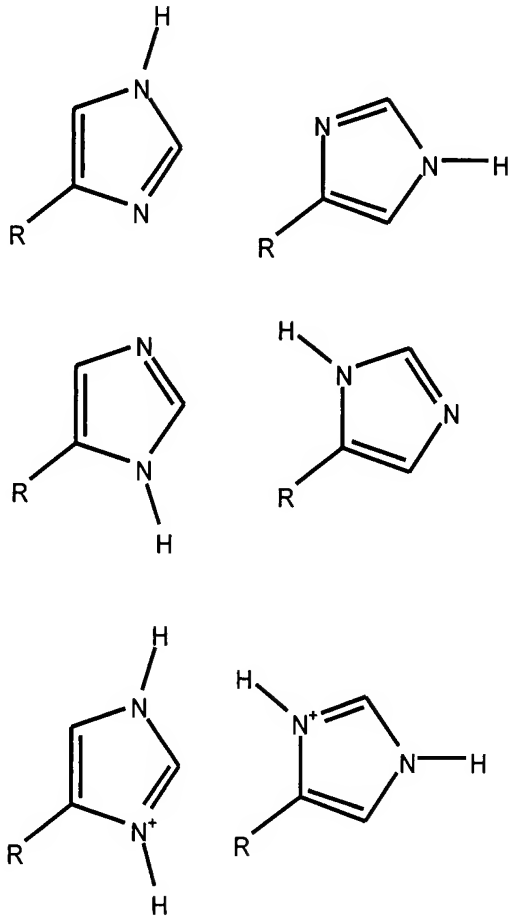
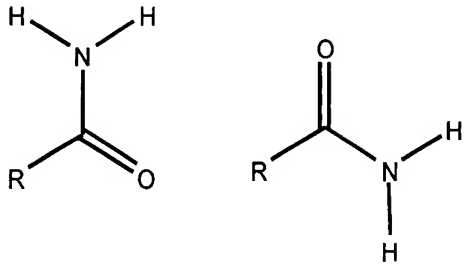

800
802
804
806
Virtual Representation Database
Virtual Representation Engine
Output Module

FIG. 8

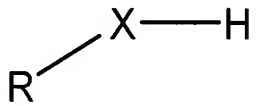
Histidine Termini
(4 neutral conformers, 2 protonated conformers, as appropriate)



Asparagine & Glutamine Residue Termini
(two conformations as shown below)



Tyrosine, Serine, Cysteine, Threonine Termini
(multiple rotor states around the R-X bond)



X = O, S

The R in each case is the remainder of specific residue under study.

FIG. 9